Understanding Propyl-cyanide and its isomers Formation: Ab initio Study of the Reaction Kinetics

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A variety of molecules (180) have been detected in the interstellar medium (ISM) [1]. Many are organic with carbon backbone. Iso-propyl cyanide (i-C_3H_7CN) a branched alkyl molecule was recently observed [2] in the ISM. The molecule was detected in a giant gas cloud called Sagittarius B2, an active region of ongoing star formation in the centre of the Milky Way. Its abundance is 0.4 times higher than its straight-chain structure isomer, suggests that branched molecules may be generally abundant in the ISM. Propyl cyanide (C_3H_7CN) is the smallest alkyl cyanide that exists in several distinct isomers. i-propyl cyanide is the largest and most complex organic molecule found to date - and the only one to share the branched atomic backbone of amino acid: some of the building blocs of life.

However the routes leading to the formation of the different propyl cyanide isomers are not clear. There is a need to accurately determine the energetics, reaction barriers, and ultimately rate constants for such complex chemistry processes, in gas and on the icy mantle of dust grains. Our goal in this work is to understand the physical and chemical processes by which new complex organic molecules such as i-C_3H_7CN and n-C_3H_7CN form in the interstellar medium. We investigated the different reaction paths for their formation routes from ab initio, and kinetic calculations points of view. We considered the gas phase formation of the propyl-cyanide isomers from the bimolecular reaction of HCN with CH_3CHCH_2. The considered mechanism involves two-step reaction for each isomer.

We employed UCCSD(T)/aug-cc-pVTZ//UMP2(full)/aug-cc-pVTZ methodology to predict the structure of the formed species and the reaction energetics. Rate constants including quantum effects were calculated for the [200-2000K] temperature range.

References

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Scientific Theme(s)
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